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* * * * * Welcome to STN International * * * * *

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NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 DEC 23 New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
USPAT2
NEWS 4 JAN 13 IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 5 JAN 13 New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
INPADOC
NEWS 6 JAN 17 Pre-1988 INPI data added to MARPAT
NEWS 7 JAN 17 IPC 8 in the WPI family of databases including WPIFV
NEWS 8 JAN 30 Saved answer limit increased
NEWS 9 FEB 21 STN AnaVist, Version 1.1, lets you share your STN AnaVist
visualization results
NEWS 10 FEB 22 The IPC thesaurus added to additional patent databases on STN
NEWS 11 FEB 22 Updates in EPFULL; IPC 8 enhancements added
NEWS 12 FEB 27 New STN AnaVist pricing effective March 1, 2006
NEWS 13 FEB 28 MEDLINE/LMEDLINE reload improves functionality
NEWS 14 FEB 28 TOXCENTER reloaded with enhancements
NEWS 15 FEB 28 REGISTRY/ZREGISTRY enhanced with more experimental spectral
property data
NEWS 16 MAR 01 INSPEC reloaded and enhanced
NEWS 17 MAR 03 Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 18 MAR 08 X.25 communication option no longer available after June 2006
NEWS 19 MAR 22 EMBASE is now updated on a daily basis
NEWS 20 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 21 APR 03 Bibliographic data updates resume; new IPC 8 fields and IPC
thesaurus added in PCTFULL
NEWS 22 APR 04 STN AnaVist \$500 visualization usage credit offered
NEWS 23 APR 12 LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 24 APR 12 Improved structure highlighting in FQHIT and QHIT display
in MARPAT
NEWS 25 APR 12 Derwent World Patents Index to be reloaded and enhanced during
second quarter; strategies may be affected

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
<http://download.cas.org/express/v8.0-Discover/>

NEWS HOURS STN Operating Hours Plus Help Desk Availability
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Enter NEWS followed by the item number or name to see news on that

10611539.trn

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:23:48 ON 13 APR 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:23:59 ON 13 APR 2006

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8

DICTIONARY FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

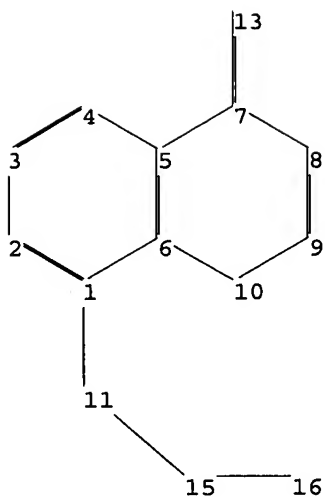
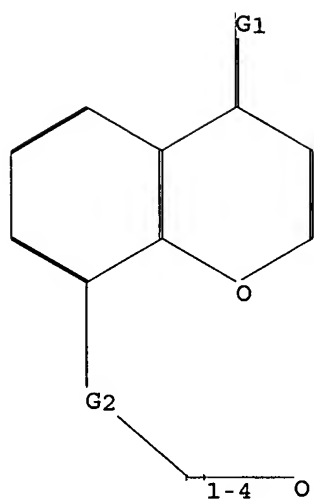
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10611539\Struc 1.str

10611539.trn



```

chain nodes :
11 13 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
1-11 7-13 11-15 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-11 5-7 6-10 7-8 7-13 8-9 9-10 11-15 15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

G1:O,S

G2:Cb,Cy,Hy

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 13:CLASS 15:CLASS 16:CLASS

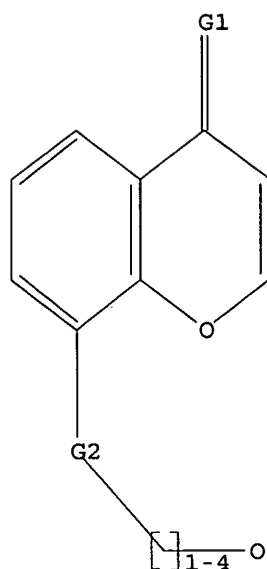
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 O,S

G2 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> l1

SAMPLE SEARCH INITIATED 15:24:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 24238 TO ITERATE

8.3% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

2 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 475446 TO 494074
PROJECTED ANSWERS: 189 TO 779

L2 2 SEA SSS SAM L1

=> l1 full

FULL SEARCH INITIATED 15:24:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 486164 TO ITERATE

100.0% PROCESSED 486164 ITERATIONS
SEARCH TIME: 00.00.05

933 ANSWERS

L3 933 SEA SSS FUL L1

=> file medline caplus
COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 166.94 | 167.15 |

FULL ESTIMATED COST

FILE 'MEDLINE' ENTERED AT 15:24:26 ON 13 APR 2006

10611539.trn

FILE 'CAPLUS' ENTERED AT 15:24:26 ON 13 APR 2006
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=> 13

L4 2661 L3

=> dup rem 14

PROCESSING IS APPROXIMATELY 74% COMPLETE FOR L4

PROCESSING COMPLETED FOR L4

L5 2494 DUP REM L4 (167 DUPLICATES REMOVED)

=> d ibib abs hitstr 2480-2494

L5 ANSWER 2480 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1940:24706 CAPLUS

DOCUMENT NUMBER: 34:24706

ORIGINAL REFERENCE NO.: 34:3816a-b

TITLE: Diuretic action of various flavone compounds,
 especially scoparin

AUTHOR(S): Clerc, A.; Paris, R.

SOURCE: Comptes Rendus des Seances de la Societe de Biologie
 et de Ses Filiales (1940), 133, 49-50
 CODEN: CRSBAW; ISSN: 0037-9026

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

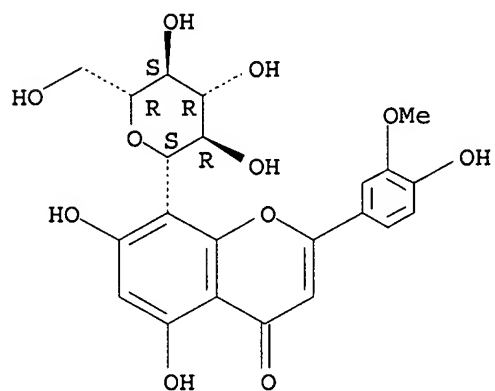
AB Scoparin (scoparoside), m. 228°, the yellow pigment of broom
 flowers (*Sarothamnus scoparius* Koch) produces marked diuresis when 1
 mg./kg. is injected into dogs. It has no significant action on the heart.
 The flavone heterosides, rutin, quercitrin, hesperidin and naringin, and
 the flavonols, scoparol and quercitol, also have a diuretic action when
 injected intravenously.

IT 301-16-6, Scoparin
 (diuretic action of)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-
 hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2481 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

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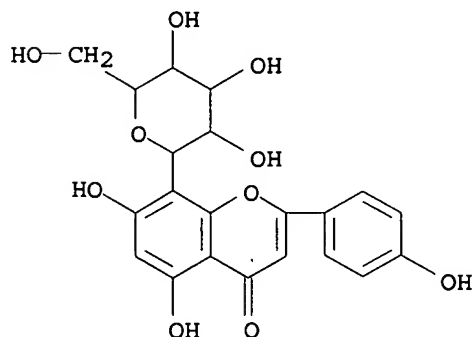
ACCESSION NUMBER: 1940:4709 CAPLUS
 DOCUMENT NUMBER: 34:4709
 ORIGINAL REFERENCE NO.: 34:764g-i
 TITLE: Vitexin
 AUTHOR(S): Peteri, Ervin
 SOURCE: Journal of the Chemical Society (1939) 1635-7
 CODEN: JCSOA9; ISSN: 0368-1769
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB Vitexin (I) was isolated by Perkin (J. Chemical Society 73, 1019 (1898); 77, 416(1900)) from New Zealand dyewood (*Vitex littoralis*) and by Barger (J. Chemical Society 89, 1210 (1906)) from *Saponaria officinalis*. P. assigned the formula C₁₅H₁₄O₇ or C₁₇H₁₆O₈ to I. I isolated by P.'s method has the formula C₁₅H₁₄O₇ and m. 263°; it yields a penta-Ac derivative, m. 251-6°. Attempts to convert I to apigenin (C₁₅H₁₀O₅) by dehydrating agents failed. Oxidation with H₂O₂ gives p-HOC₆H₄CO₂H (II) and a minute quantity of quinol; Fehling solution gives 1,3,5-C₆H₃(OH)₃, p-HOC₆H₄Ac and an amorphous acid; K₃Fe(CN)₆ gives II. I reduces a large amount of AgNO₃-NH₄OH but the oxidation product could not be isolated; it does not react with Pb(OAc)₄ in AcOH, possibly owing to its insoly. I does not yield crystalline compds. with the usual methylating agents. Nitration of I and crystallization from dioxane gives the tetra-NO₂ derivative, yellow, m. 257°, which does not depress the m. p. of tetranitroapigenin. Sublimation of I with Zn dust at 350-60° gives a compound C₁₅H₁₂O₆, the Ac derivative of which does not depress that of triacetylapiogenin (m. 181-2°).

IT 3681-93-4, Vitexin
 (and derivs.)

RN 3681-93-4 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 2482 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1937:44787 CAPLUS
 DOCUMENT NUMBER: 31:44787
 ORIGINAL REFERENCE NO.: 31:6245h-i
 TITLE: The constitution of the scoparoside (scoparin) of *Sarothamnus scoparius* Koch
 AUTHOR(S): Mascre, Marcel; Paris, Rene
 SOURCE: Compt. rend. (1937), 204, 1581-3
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB cf. C. A. 31, 4983.8. Scoparoside is a heteroside, C₂₂H₂₂O₁₁.H₂O, difficultly hydrolyzed, but can be hydrolyzed by the enzyme

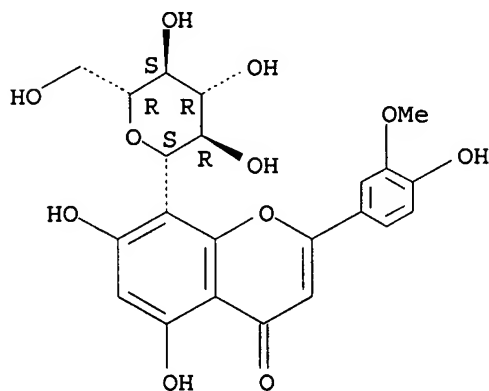
rhamnodiastase, giving 1 mol. of rhamnose, C₆H₁₂O₅; and 1 mol. of scoparol, C₁₆H₁₂O₇, the latter being flavone derivative, probably a Me ether of quercitol.

IT 301-16-6, Scoparin
(preparation of)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2483 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1937:35350 CAPLUS

DOCUMENT NUMBER: 31:35350

ORIGINAL REFERENCE NO.: 31:4983h-i,4984a

TITLE: Scoparin (scoparoside) of *Sarothamnus scoparius* Koch

AUTHOR(S): Mascré, Marcel; Paris, René

SOURCE: Compt. rend. (1937), 204, 1270-1

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

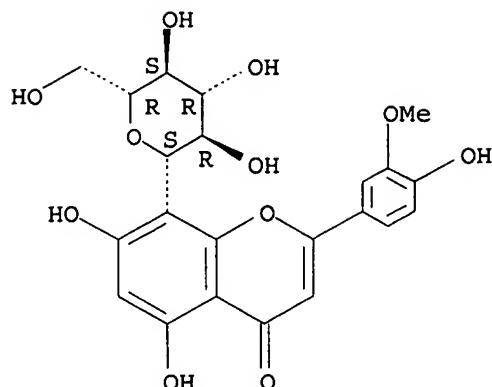
AB The following method was used for the preparation of pure scoparin (I) in 1-1.2% yield. The flowers of *Sarothamnus scoparius* were extracted with boiling 90% alc. and the concentrated extract was taken up in boiling H₂O and filtered. When the filtrate was washed with Et₂O and chilled, a clear brown gelatinous mass separated. This was dissolved in boiling anhydrous EtOAc. On cooling crystals of I separated which were washed with Et₂O, dried over H₂SO₄, and recrystd. from EtOAc or 80% EtOH. I is little soluble in cold and somewhat more soluble in hot H₂O, EtOH, AmOH, HOAc, EtOAc, AcH and C₅H₅N, insol. in Et₂O, CHCl₃ and C₆H₆. It dissolves in the presence of alkalies, giving deep yellow solns., and is repptd. on acidification with partial decolorization. From aqueous solution I is precipitated with Pb(OH)OAc. It reduces

Fehling solution slightly. I contains no ash or N. At 100° it loses 7% of its weight and in vacuo at 60° 7.22%. The composition is represented by the formula C₂₂H₂₂O₁₁·2H₂O. I m. 230°. M. and P. consider I to be a heteroside composed of 1 methylpentose and 1 flavone residue which is difficult to hydrolyze. The pure product does not possess the diuretic properties usually attributed to scoparin.

IT 301-16-6, Scoparin
(preparation of)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1938:4681 CAPLUS

DOCUMENT NUMBER: 32:4681

ORIGINAL REFERENCE NO.: 32:726a-d

TITLE: Scoparoside (scoparine) from *Sarothamnus scoparius*
Koch

AUTHOR(S) : Mascre, M.; Paris, R.

SOURCE: Bulletin des Sciences Pharmacologiques (1937), 44, 401-15

CODEN: BSPHAV; ISSN: 0366-3493

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 31, 6245.9. Scoparine was prepared either by the method of Stenhouse, or by extraction with AcOH and precipitation with Et2O. Fresh flowers give

a better yield than the dry drug. Scoparine m. at 228-230° decomposition It is of very low solubility in cold H₂O, insol. in Et₂O, CHCl₃

and

PhH, easily soluble in alcs. and Me₂CO. It reduces Fehling solution at 100°. When dried at 100° or at 60° in vacuo, it loses 7.22% equivalent to 2H₂O. The formula C₂₂H₂₂O₁₁·2H₂O was confirmed.

Hydrolysis with 10% KOH forms the following cleavage products:

acetovanillone, 4-Ac-C6H3OH-2-MeO, vanillic acid and protocatechuic acid. Acid hydrolysis does not attack the mol. sufficiently to produce identifiable split products. Methylfurfurole was formed in small quantities. The action of rhamnodiastase from the seeds of *Rhamnus utilis*

splits off a sugar, supposed to be rhamnose. Scoparine is considered to be a heteroside and a change of the name to scoparoside is suggested.

After the separation of rhamnose, scoparol, C16H12O7, the Me ether of quercetol would be formed. The substance is of very low toxicity; exact determination is impossible because of insufficient solubility. The pure substance produces in the anesthetized dog a temporary drop in blood pressure, a slight decrease in size of the kidney and a passing decrease of diuresis. The crude drug, which is far more soluble, produces secondarily an increase in kidney size and increased diuresis. The difference in action can be due either to the higher solubility or to impurities.

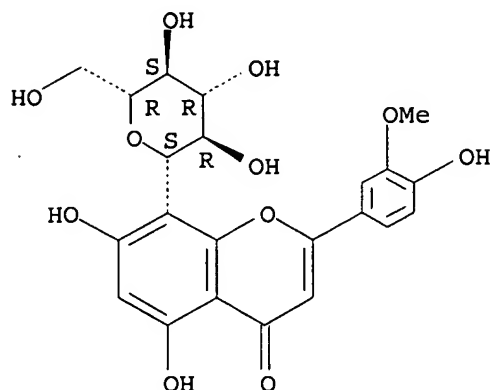
IT 301-16-6, Scoparin
(from *Sarothamnus scoparius*)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-

hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

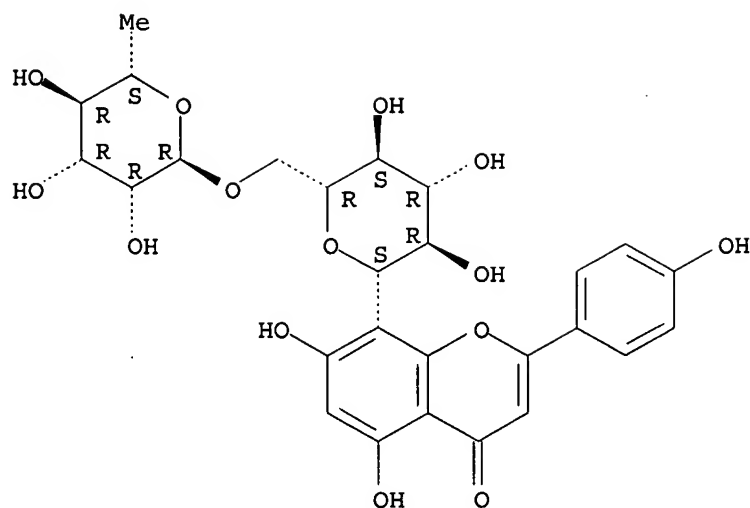
Absolute stereochemistry.



L5 ANSWER 2485 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1934:1123 CAPLUS
 DOCUMENT NUMBER: 28:1123
 ORIGINAL REFERENCE NO.: 28:175c-d
 TITLE: Compounds of the "abietene family"
 INVENTOR(S): Henke, Clyde O.; Charlton, Malcolm
 PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| | ----- | ---- | ----- | ----- | ----- |
| | US 1931257 | | 19331017 | US 1931-540010 | 19310525 |
| AB | A sulfonic derivative of abietene, abietine or abietane is condensed with an aldehyde such as formaldehyde or benzaldehyde or a compound of like reactivity such as paraformaldehyde or benzal chloride to form a product which may be used as a wetting, dispersing or tanning agent. | | | | |
| IT | 54302-43-1, Abietin (derivs.) | | | | |
| RN | 54302-43-1 CAPLUS | | | | |
| CN | 4H-1-Benzopyran-4-one, 8-[6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME) | | | | |

Absolute stereochemistry.



L5 ANSWER 2486 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1935:19193 CAPLUS

DOCUMENT NUMBER: 29:19193

ORIGINAL REFERENCE NO.: 29:2448i,2449a

TITLE: Absorption spectra of colored organic salts of violantin and alloxantin

AUTHOR(S): Gaind, K. N.; Dutt, S.

SOURCE: Bull. Acad. Sci. United Provinces Agra Oudh, Allahabad (1933), 3, 79-82

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

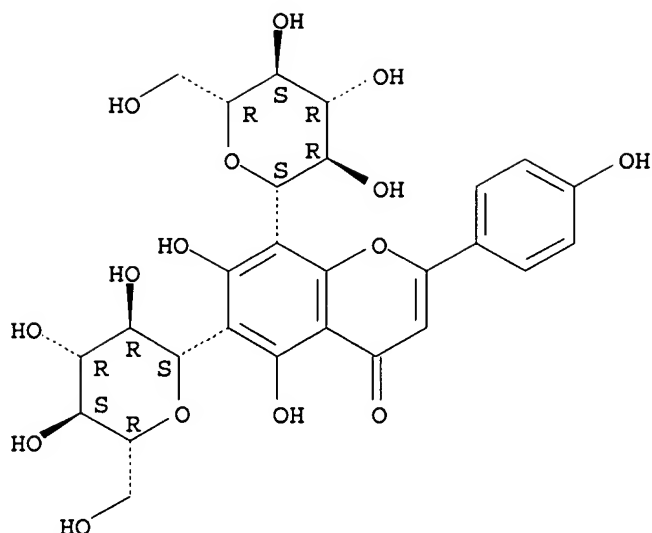
AB The positions of the absorption maxima for a number of salts of these compds. are tabulated.

IT 23666-13-9, Violantin
(spectra of colored organic salts of)

RN 23666-13-9 CAPLUS

CN 4H-1-Benzopyran-4-one, 6,8-di-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2487 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1927:4596 CAPLUS
 DOCUMENT NUMBER: 21:4596
 ORIGINAL REFERENCE NO.: 21:575c-d
 TITLE: Scoparin
 AUTHOR(S): Hemmelmayr, Franz; Strehly, Josefine
 SOURCE: Monatshefte fuer Chemie (1926), 47, 379-92
 CODEN: MOCMB7; ISSN: 0026-9247
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

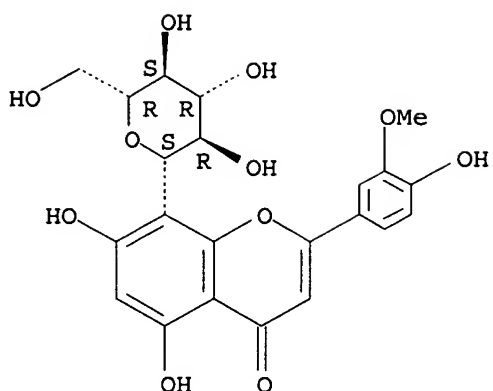
AB Scoparin is assigned the formula C₂₂H₂₃O₁₁ (cf. Herzig and Tiring, C. A. 13, 421). The difficultly soluble modification, first observed by Stenhouse (Ann. 78, 15) by the action of EtOH, also results with MeOH. K compound, C₂₂H₁₅O₁₁K₇, ppts. on addition of EtOH to a solution in 40% KOH. The Na compound appears to contain only 6 Na, while the Ba compound analyzes for C₄₄H₃₆O₂₂Ba₄. It is not possible completely to methylate or ethylate scoparin. It appears to yield a pentachloroacetyl derivative, yellow; this is soluble in KOH with a yellow color, indicating at least 1 free HO group. Heptaanisoyl derivative(?), m. 135°. Boiling dilute H₂SO₄ appears to form at first an isomeric scoparin and then gradually splits off H₂O. Boiling dilute HCl gives a compound containing 2 mols. H₂O less than scoparin.

IT 301-16-6, Scoparin
 (and derivs.)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2488 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1924:16033 CAPLUS

DOCUMENT NUMBER: 18:16033

ORIGINAL REFERENCE NO.: 18:2131c-f

TITLE: 5-Nitrobarbituric acids

AUTHOR(S): Biltz, Heinrich; Sedlatscheck, Kurt

SOURCE: Ber. (1924), 57B, 339-49

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB 5-Nitrobarbituric acid (I), decomp. 180-1°, is obtained in 95% yield by nitrating violuric acid, decomp. 240-1°. Treated with Cl in aqueous suspension until solution results, there is formed the 5-Cl derivative,

decomp. 86-7°, which is decomposed by warm H₂O into I, CCl₃NO₂ and CO(NH₂)₂ and by bleaching powder into CO(NH₂)₂ and CCl₃NO₂. 5-Br derivative, decomp. 108°, and behaves towards H₂O as the Cl derivative. Methylvioluric acid gives 92° of 1-methyl-5-nitrobarbituric acid (II), crystallizing with 2H₂O, decomposing 142-3°. NH₄ salt, fine needles, stable at 120°; K salt, fine needles; Na salt, needles with 1 H₂O; Ba salt, needles with 1 H₂O; the acid is stable towards alkalis. 5-Cl derivative, decomp. 122-3°; it is decomposed by H₂O into II, MeNHCONH₂, CCl₃NO₂ and CO₂. 5-Br derivative, decomp. 137-8°. 1,3-Dimethyl-5-nitrobarbituric acid, decomp. 148-9° (95% yield); Na salt, yellow needles with 4H₂O. The 5-Cl derivative, decomp. 150° (Andreasch, Monatsh. 16, 786, observed no decomposition at 250°). The 5-Br derivative decomp. 152° (A. gives m. partially 152°). These same derivs. are obtained by the action of CH₂N₂ upon the corresponding derivs. of I, thus establishing the position of the halogen. 1-Ethyl-5-nitrobarbituric acid, needles with 1 H₂O, decomp. 132-3°; NH₄ salt, needles, stable at 120°; K salt, yellow needles; Na salt, yellow needles with 1 H₂O; Ca salt, needles; Sr salt, prisms with 1 H₂O. The 5-Cl derivative decomp. 127-8°, the 5-Br derivative at 138-9°. 1,3-Diethyl-5-nitrobarbituric acid decomp. 116-7°; this is also obtained in 32° yield by the direct nitration of 1,3-diethylbarbituric acid. NH₄ salt, long needles, stable at 120°. 5-Cl derivative, decomp. 53°. 5-Br derivative decomp. 63-4°. Violantin and its alkyl derivs. (Baeyer, Ann. 127, 223) do not exist.

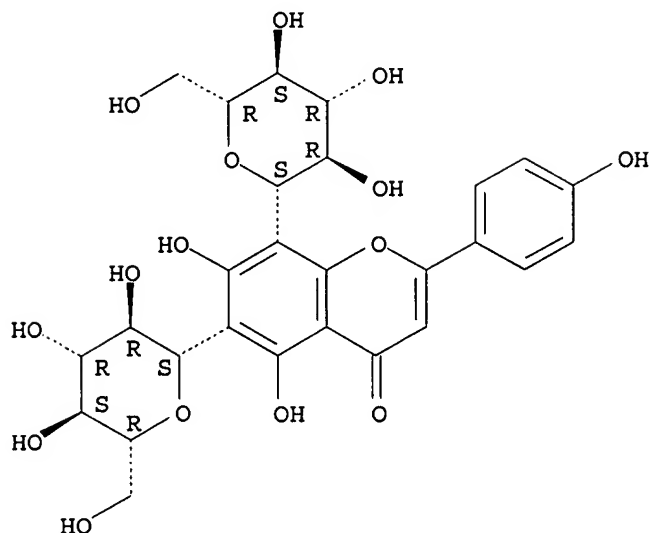
IT 23666-13-9, Violantin
(and alkyl derivs., nonexistence of)

RN 23666-13-9 CAPLUS

CN 4H-1-Benzopyran-4-one, 6,8-di-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-

hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2489 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1919:2492 CAPLUS

DOCUMENT NUMBER: 13:2492

ORIGINAL REFERENCE NO.: 13:421c-e

TITLE: Scopolamine

AUTHOR(S): Herzig, J.; Tieing, Gertrud

SOURCE: Journal of the Chemical Society, Abstracts (1918), 114(I), 503

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

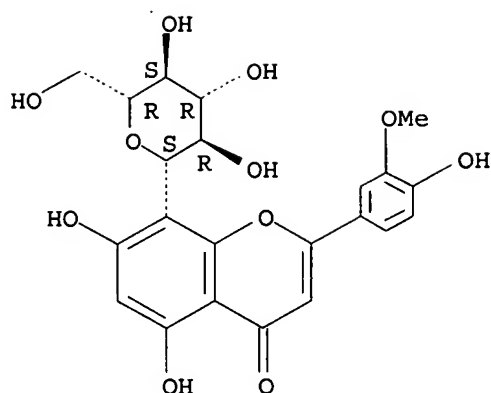
AB Goldschmiedt and von Hemmelmayer have shown that scopolamine obtained from *Spartium scopolarium* contains a MeO group and 6 HO radicals and attributed to the substance the formula $C_{20}H_{20}O_{10}$; it was found possible to alkylate only 1 HO radical. By using CH_2N_2 , however, it is possible to obtain a dimethyl derivative (trimethylnorscopolamine), $C_{24}H_{28}O_{12}$, yellow crystals, m. $260-5^\circ$ (decomposition), and a trimethyl derivative (tetramethylnorscopolamine), $C_{25}H_{30}O_{12}$, yellow crystals, m. $220-38^\circ$, together with an amorphous substance. With MeI and Ag_2O , it is possible to convert scopolamine into a crystalline octamethylnorscopolamine, $C_{21}H_{12}O_3(OMe)_8$, m. $120-30^\circ$, with subsequent resolidification and m. $229-33^\circ$. The composition of these substances, as also that of acetylscopolamine, renders it probable that the mol. formula of scopolamine is not $C_{20}H_{20}O_{10}$, but $C_{22}H_{22}O_{11}$.

IT 301-16-6, Scopolamine
(and derivs.)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8- β -D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2490 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1919:2490 CAPLUS

DOCUMENT NUMBER: 13:2490

ORIGINAL REFERENCE NO.: 13:420f-i,421a-c

TITLE: Binuclear quinones. Chemical action of light

AUTHOR(S): Meyer, Hans; Eckert, Alfred

SOURCE: Journal of the Chemical Society, Abstracts (1918), 114(II), 385-6

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

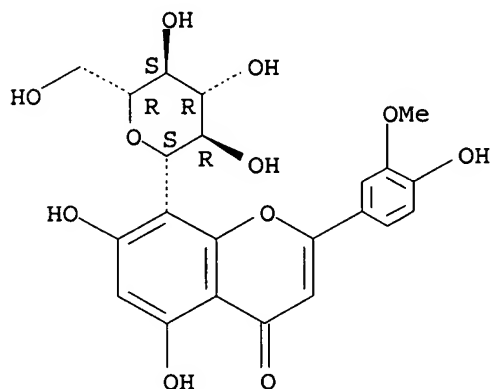
LANGUAGE: Unavailable

AB Meyer and Hofmann have shown that dihydroanthracene, when heated, readily decomps. into anthracene and H, and it is therefore to be expected that the same dissociation should occur under the influence of light. Contrary to the statement of Orndorff and Cameron, this substance does undergo chemical alteration when exposed to light from the sun or elec. arc, the products being H and para-anthracene, the latter being formed by the immediate polymerization of the "nascent" anthracene, which is the primary product. In the presence of substances capable of reacting with this "nascent" anthracene, other products may be obtained. The action of light on anthracene probably also gives rise to "nascent" anthracene in which the diagonal valency becomes resolved into 2 free valencies. By these the formation of para-anthracene becomes possible. If O is present, the products are anthraquinone and dihydrodianthrone, the latter being formed by the further action of light on anthranol, which represents an intermediate stage of the change. It is already known that solns. of benzoquinone and thymoquinone in EtOH when subjected to light give rise to AcH and the corresponding quinol. With anthraquinone, however, the quinol derivative is unstable, and in contact with air regenerates anthraquinone; it is therefore possible to use anthraquinone as a catalyst for the oxidation of EtOH to AcH in light, the only other product being a small quantity of an unidentified substance which gives a brown solution in aqueous KOH. In a similar manner iso-PrOH can be oxidized to acetone, but MeOH is very stable and is recovered completely unchanged, together with the anthraquinone. This relative stability of MeOH accords well with the earlier results of Meyer and Hofmann and may account for the preponderance of Me derivs. among the naturally occurring alkyl compds. 9,10-Dichloro- and 9,10-dibromoanthracene are unaffected by light but 10-bromoanthracene in alc. gradually gives rise to anthraquinone and Br ions, together with a temporary small deposit of para-anthracene. If dihydroanthracene in Ac₂O is submitted to the action of light, the 1st deposit of para-anthracene may disappear on prolonged treatment, probably

by further oxidation to anthraquinone. Anthranyl acetate is obtained as a by-product, its formation supplying an explanation of the origin of dihydroanthracene in the action of light and air on anthracene in alc. solution. Solns. of anthracene in AcOH, CHCl₃ and Me₂SO₄, when illuminated, give the same products; it was hoped with the aid of Me₂SO₄ to isolate anthraquinol in the form of the di-Me ether, but unfortunately this compound is sensitive to light and in AcOH is rapidly converted into anthraquinone.

IT 301-16-6, Scoparin
(and derivs.)
RN 301-16-6 CAPLUS
CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

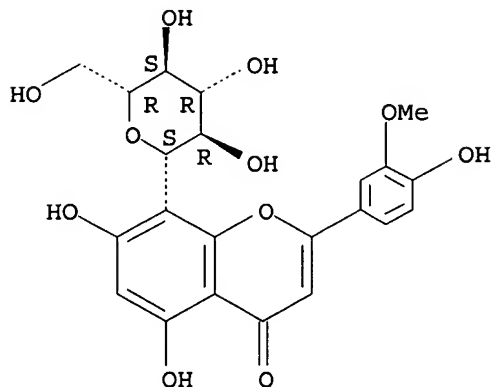


L5 ANSWER 2491 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1919:2491 CAPLUS
DOCUMENT NUMBER: 13:2491
ORIGINAL REFERENCE NO.: 13:421c-e
TITLE: Scoparin
AUTHOR(S): Herzig, J.; Tieing, Gertrud
SOURCE: Monatshefte fuer Chemie (1918), 39, 253-67
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Goldschmiedt and von Hemmelmayr have shown that scoparin obtained from Spartium scoparium contains a MeO group and 6 HO radicals and attributed to the substance the formula C₂₀H₂₀O₁₀; it was found possible to alkylate only 1 HO radical. By using CH₂N₂, however, it is possible to obtain a dimethyl derivative (trimethylnorscoparin), C₂₄H₂₈O₁₂, yellow crystals, m. 260-5° (decomposition), and a trimethyl derivative (tetramethylnorscoparin), C₂₅H₃₀O₁₂, yellow crystals, m. 220-38°, together with an amorphous substance. With MeI and Ag₂O, it is possible to convert scoparin into a crystalline octamethylnorscoparin, C₂₁H₁₂O₃(OMe)₈, m. 120-30°, with subsequent resolidification and m. 229-33°. The composition of these substances, as also that of acetylseoparin, renders it probable that the mol. formula of scoparin is not C₂₀H₂₀O₁₀, but C₂₂H₂₂O₁₁.

IT 301-16-6, Scoparin
(and derivs.)
RN 301-16-6 CAPLUS
CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2492 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1919:2489 CAPLUS
 DOCUMENT NUMBER: 13:2489
 ORIGINAL REFERENCE NO.: 13:420f-i,421a-c
 TITLE: Binuclear quinones. Chemical action of light
 AUTHOR(S): Meyer, Hans; Eckert, Alfred
 SOURCE: Monatshefte fuer Chemie (1918), 39, 241-51
 CODEN: MOCMB7; ISSN: 0026-9247
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB Meyer and Hofmann have shown that dihydroanthracene, when heated, readily decomps. into anthracene and H, and it is therefore to be expected that the same dissociation should occur under the influence of light. Contrary to the statement of Orndorff and Cameron, this substance does undergo chemical alteration when exposed to light from the sun or elec. arc, the products being H and para-anthracene, the latter being formed by the immediate polymerization of the "nascent" anthracene, which is the primary product. In the presence of substances capable of reacting with this "nascent" anthracene, other products may be obtained. The action of light on anthracene probably also gives rise to "nascent" anthracene in which the diagonal valency becomes resolved into 2 free valencies. By these the formation of para-anthracene becomes possible. If O is present, the products are anthraquinone and dihydrodianthrone, the latter being formed by the further action of light on anthranol, which represents an intermediate stage of the change. It is already known that solns. of benzoquinone and thymoquinone in EtOH when subjected to light give rise to AcH and the corresponding quinol. With anthraquinone, however, the quinol derivative is unstable, and in contact with air regenerates anthraquinone; it is therefore possible to use anthraquinone as a catalyst for the oxidation of EtOH to AcH in light, the only other product being a small quantity of an unidentified substance which gives a brown solution in aqueous KOH. In a similar manner iso-PrOH can be oxidized to acetone, but MeOH is very stable and is recovered completely unchanged, together with the anthraquinone. This relative stability of MeOH accords well with the earlier results of Meyer and Hofmann and may account for the preponderance of Me derivs. among the naturally occurring alkyl compds. 9,10-Dichloro- and 9,10-dibromoanthracene are unaffected by light but 10-bromoanthracene in alc. gradually gives rise to anthraquinone and Br ions, together with a temporary small deposit of para-anthracene. If dihydroanthracene in Ac2O is submitted to the action of light, the 1st

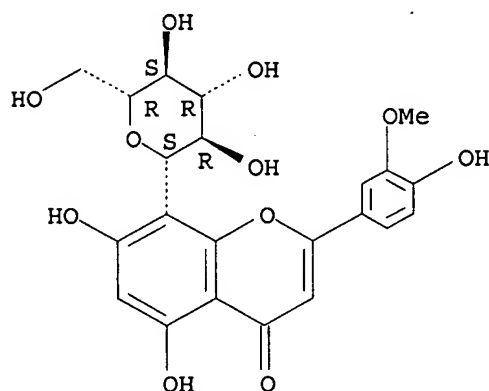
deposit of para-anthracene may disappear on prolonged treatment, probably by further oxidation to anthraquinone. Anthranyl acetate is obtained as a by-product, its formation supplying an explanation of the origin of dihydroanthracene in the action of light and air on anthracene in alc. solution. Solns. of anthracene in AcOH, CHCl₃ and Me₂SO₄, when illuminated, give the same products; it was hoped with the aid of Me₂SO₄ to isolate anthraquinol in the form of the di-Me ether, but unfortunately this compound is sensitive to light and in AcOH is rapidly converted into anthraquinone.

IT 301-16-6, Scoparin
(and derivs.)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2493 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1919:1306 CAPLUS

DOCUMENT NUMBER: 13:1306

ORIGINAL REFERENCE NO.: 13:216e-g

TITLE: Action of the potassium ferricyanide and ferric chloride reagent on alkaloids, glucosides and other plant constituents

AUTHOR(S): Palet, Luciano P. J.

SOURCE: Anales soc. quim. Argentina (1918), 6, 156-8

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

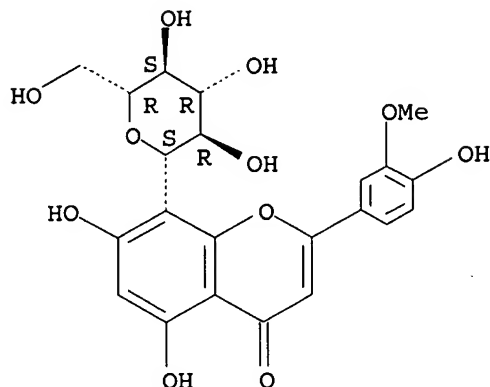
AB P. tested the action of the K₃Fe(CN)₆-Fe₂(Cl)₆ reagent (cf. preceding abstract) on 102 plant constituents. A positive reaction was given by the following alkaloids: apomorphine, beberine, berberine, brucine, codeine, colchicine, curarine, emetine, sparteine, erythrofleine, physostygmine, hydrastine, morphine, meconine, napeline, narcotine, pelletierine, pseudopelletierine, pereirine, sabadilline. A positive reaction was obtained with the following glucosides: adonidin, apocinin, arbutin, apiin, boldin, convalamarin, esculin, strophanthin, smilacin, floricin, globularin, graciolin, helleborin, hesperidin, sabatin, salicin, sapotoxin, siringuin. A positive reaction was obtained with the following bitter principles: aloin, cotoina verum, scoparin.

IT 301-16-6, Scoparin
(reaction with K₃Fe(CN)₆-Fe₂Cl₆ reagent)

RN 301-16-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2494 OF 2494 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1907:159 CAPLUS
 DOCUMENT NUMBER: 1:159
 ORIGINAL REFERENCE NO.: 1:54c-g
 TITLE: American Colophonium
 AUTHOR(S): Levy, Paul
 CORPORATE SOURCE: Organic Lab., Tech. High School of Aachen
 SOURCE: Ber. (1907), 39, 3043-46
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

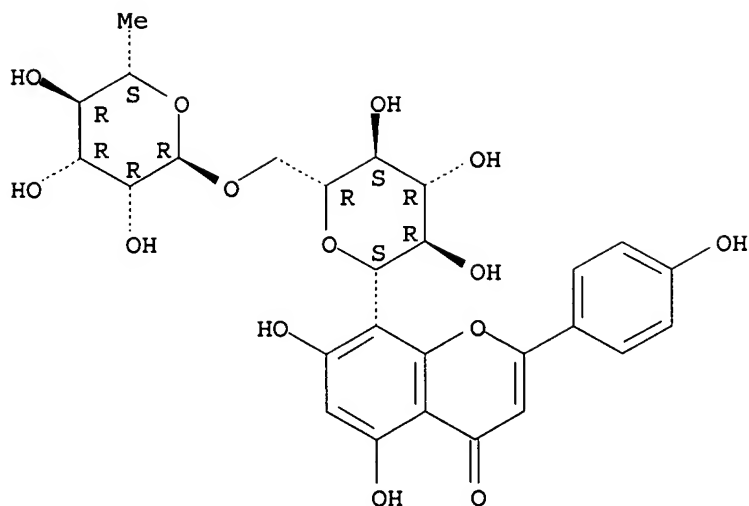
AB The author has already shown (Z. angew. Chemical, 18, 1739, (1905)) that abietic acid is obtained in excellent yield and in a high degree of purity by the distillation of American colophonium. His preparation differs from those of other workers in its higher melting point and pronounced crystallizing power. Measurements show that it forms monoclinic sphenoids, identical with other preparations. With phosphorus pentachloride or thionyl chloride, it yields an acid chloride, which could not be purified. When distilled this decomposes into hydrogen chloride, carbon monoxide, and "abietin," C₁₉H₂₈. Colorless, oily liquid, 17b 200°-202°. It has an intense blue fluorescence and appears to be identical with a compound obtained by Kraemer and Spilker (Ber., 32, 2953, 3614 (1899), by the dry distillation of colophonium. Another hydrocarbon, C₁₉H₃₀, is obtained, together with abietic acid by the distillation of American colophonium. Colorless oil, 26.5b 210°. 211°, sp. gr. = 0.977 at 20°. It shows feeble refractive power and is identical with Deville's "colophene," C₁₀H₆₄. (Ann., 37, 193, 1841) with Bischoff and Nastvogel's (Ber., 23, 1919, (1890)), compound, C₂₀H₃₂, and with Easterfield and Bagley's "albietene," C₁₈H₈₈. (J. Chemical Society, 85, 1238, (1904)). It is formed from abietic acid by the elimination of carbon dioxide.

IT 54302-43-1, Abietin
 (preparation of)

RN 54302-43-1 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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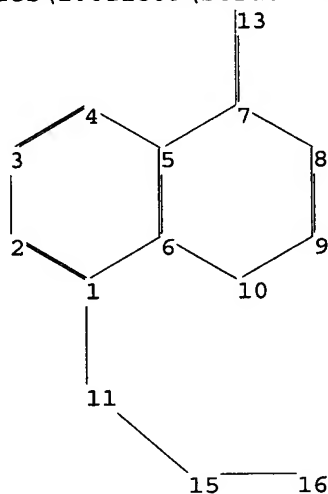
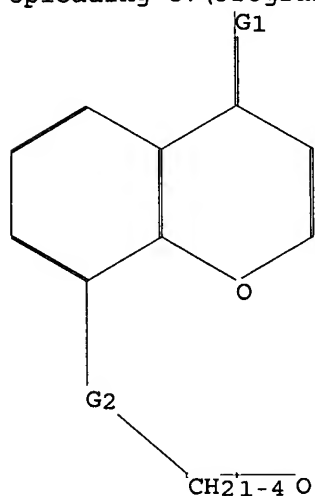
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chain nodes :

11 13 15 16

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-11 7-13 11-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

1-11 5-7 6-10 7-8 7-13 8-9 9-10 11-15

exact bonds :

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normalized bonds :

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G1:O,S

G2:Cb,Cy,Hy

Match level :

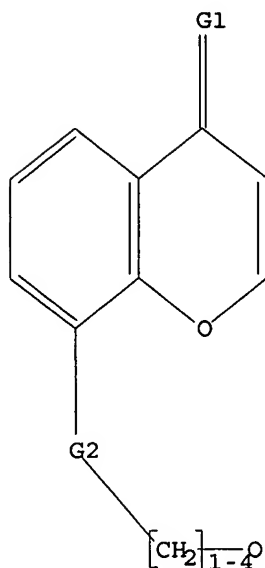
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11:CLASS 13:CLASS 15:CLASS 16:CLASS

L6 STRUCTURE UPLOADED

10611539.trn

=> d
L6 HAS NO ANSWERS
L6 STR



G1 O,S
G2 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 24238 TO ITERATE

8.3% PROCESSED 2000 ITERATIONS 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 475446 TO 494074
PROJECTED ANSWERS: 189 TO 779

L7 2 SEA SSS SAM L6

=> 16 full
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FULL SCREEN SEARCH COMPLETED - 486164 TO ITERATE

100.0% PROCESSED 486164 ITERATIONS 727 ANSWERS
SEARCH TIME: 00.00.04

L8 727 SEA SSS FUL L6

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 L10 2477 DUP REM L9 (167 DUPLICATES REMOVED)

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